Anti-correlation between energy-gap and phonon energy for cuprate Bi2212 superconductor

Wei Fan
Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, 230031-Hefei, People's Republic of China
(Dated: February 1, 2008)

Using electron-phonon mechanism, we explains very well the spatial anti-correlation between the energy-gap and the energy of phonon mode for cuprate superconductor found in d^2I/dV^2 spectrum by STM measurements [Jinho Lee, et.al Nature **442**,546 (2006)], which is is the direct effect of a relationship $M\langle\omega^2\rangle\lambda = const$. We calculate T$_C$ maps on $\lambda-\Omega_P$ plane which helps us understanding the relation $M\langle\omega^2\rangle\lambda = const$ and the superconductivity of superconductors.

PACS numbers: 74.20.Fg, 74.25.Kc, 74.62.-c, 74.72.-h, 74.81.-g

Scanning Tunneling Microscopy/Spectroscopy (STM/S) has been used to explore surface structures and electronic structures of superconductors [1]. The electronic inhomogeneity such as the inhomogeneously distributed energy-gaps and local densities of states has been found in High Temperature Superconductor (HTSC) [2, 3]. The intrinsic inhomogeneity even exists when translational invariance of lattice structure preserves. If total momentum of cooper pair isn't equal zero, in real-coordinate space the distribution of cooper pairs is inhomogeneous. The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase can be realized by applying magnetic field or stress field to superconductors.

An interesting property of electronic inhomogeneity of superconductor by the observations of STM/S for HTSC Bi2212 is the spatial anti-correlations of energy-gap and energy of boson mode [3]. The understanding of origin of the anti-correlation is very useful to understand the microscopic mechanism of superconductivity for HTSC materials. The boson mode for Bi2212 has been identified as phonon mode due to the isotope effects.

The out-of-plane buckling modes, in-plane breathing modes and the phonon modes related apical oxygen atoms are expected to contribute to superconductivity of HTSC materials. The out-of-plane buckling modes coupling with the electrons near anti-node region have small momentum transfer and significant band renormalization effects near transition temperatures which had been found in ARPES spectrum and theoretical calculation [4].

In this paper, we preform the standard calculations of Nambu-Eliashberg strong coupling theory and focus on an important relation $M\langle\omega^2\rangle\lambda = \eta = const$. The superconductor parameter $\eta = \rho(0)\langle J^2\rangle$, the product of the electronic properties $\rho(0)$ the density of state at Fermi energy and the electron-phonon matrix elements J, characterizes the chemical environments of atoms and almost keeps as a constant against the simple structural changes such as the isotope substitution. We assume the electron-phonon mechanism is pairing mechanism for superconductor Bi2212 in this paper because of the isotope effects and identification of phonon mode in ARPES spectrum [6], STM/S experiments [3]. In terms of the relation $M\langle\omega^2\rangle\lambda = \eta$, we explain the anti-correlation between energy-gap Δ and phonon energy Ω_P. We also plot two T$_C$ maps of transition temperature on $\lambda-\Omega_P$ plane, which are very useful to understand superconductivity of conventional and unconventional superconductors.

The theoretical methods used in this paper are (1) the real-energy method by having analytically continued the imaginary Eliashberg Equation to real axis [7, 8] and (2) the imaginary-energy Matsubara method [9] of strong coupling superconducting theory under isotropic approximation. After having resolved isotropic energy-gap equation, we can obtained the anisotropic energy-gap by directly multiplying isotropic energy-gap $\Delta(\omega)$ with the anisotropic function such as for the d-wave the anisotropic energy-gap $\Delta(\omega)\cos(2\theta)$ and then averaging it over θ angle. The anisotropy of energy-gap comes from the anisotropic electron-phonon interaction [4, 5]. The real-energy method gives the results of densities of states, energy gaps and T$_C$. The advantage of imaginary methods is that we can quickly obtain the T$_C$ compared with the real-energy methods.

The densities of state of phonon is calculated by following formula [7]

$$F(\omega) = \begin{cases} \frac{c}{(\omega-\Omega_p)^2+(\omega_2)^2} - \frac{c}{(\omega_3)^2+(\omega_2)^2}, & |\omega-\Omega_p| < \omega_3 \\ 0 & \text{others,} \end{cases} \quad (1)$$

where Ω_p is the energy of phonon mode, ω_2 the half-width of peak of phonon mode and $\omega_3^\lambda = 2\omega_2$. The effective electron-phonon interaction $\alpha_y^2(\nu)$ is defined by

$$\alpha_y^2(\omega)F_y(\omega) = \frac{1}{W}\int_S \frac{d^{d-1}p}{v_F}\int_{S'} \frac{d^{d-1}p'}{v_{F'}} B_y(p-p',\omega)|D^e_{p-p',y}|^2. \quad (2)$$

where $W = 1/(2\pi)^{d-1}\int_S d^{d-1}p/v_F$ and v^F Fermi velocity. In 2-dimensional limit the coupling between different layers being ignored, we can solve the Eliashberg equation for 2-dimensional systems. Compared with 3-dimensional system, the energy-gap equation keeps unchanged and all changes are included in the Eliashberg function $\alpha^2F(\omega)$. Complete treatments of anisotropic effects need the k-dependent energy-gap function $\Delta(k,\omega)$ and re-normalized factors $Z(k,\omega)$.

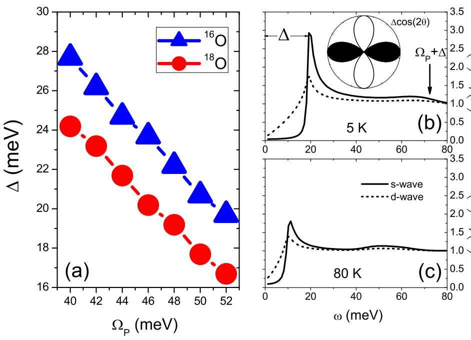

FIG. 1: (a). The anti-correlation between energy-gap Δ and the phonon energy Ω_P and corresponding isotope effects for ^{16}O substituted by ^{18}O. (b,c). The s-wave and d-wave densities of states at 5 K and 80 K. The definition of energy gap Δ by densities of states (DOS) and energy gap with d-wave symmetry in (b).

We can write the parameter of electron-phonon interaction $\lambda = \sum_y \lambda_y$, where parameter $\lambda_y = 2\int_0^\infty d\omega\alpha_y^2 F_y(\omega)/\omega$ is the contribution of y mode to total λ. The moments $\langle\omega^n\rangle$ of the distribution function $(2/\lambda)\sum_y 2\alpha_y^2 F_y(\omega)/\omega$ are defined as $\langle\omega^n\rangle = 2/\lambda\sum_y\int_0^\infty d\omega\alpha_y^2 F_y(\omega)\omega^{n-1}$. In this work we assume that α_y is constant around each peak in phonon spectrum. Under this approximation, we only consider $\alpha^2F(\omega)$ as a whole, the so-called Eliashberg function with above Lorentz shape. In practice, by modifying the height of peak of Eliashberg function $\alpha^2F(\omega)$, we can control the change of the parameter λ of electron-phonon interaction. The densities of states of electron are obtained from the formula $\rho(\omega) = \rho_N(\omega)Re(\omega/\sqrt{\omega^2-\Delta(\omega)^2})$. If the anisotropy of energy gap is considered such as with the d-wave symmetry, the density of state $\rho(\omega) = \rho_N(\omega)\langle Re(\omega/\sqrt{\omega^2-(\Delta(\omega)\cos(\theta))^2})\rangle_\theta$, with the $\langle\ldots\rangle_\theta$ describing the average over θ.

We choose the phonon spectrum of Eq. (1) with phonon-energy about Ω_P=52 meV, which is the mean phonon-energy observed in the tunneling spectrum of Bi2212 [3]. The Ω_P distributes from 30 meV to 70 meV and within the range from about 36 meV the B_{1g} phonon coupling to electrons at antinode region and to 70 meV the in-plane breathing mode coupling with electrons at node region based on the observation of ARPES spectrum [6].

If the parameter λ of electron-phonon interaction is 2.0 and the Coulomb pseudo-potential μ^*=0.24, the transition temperature T_C is about 90K close the experimental values. From STM experiments of Bi2212, the energies of phonon have a distribution with width about $2\omega_2$=16 meV. The energy gap Δ and the λ the parameter of electron-phonon interaction should have distributed with their widthes respectively. If we consider a material with multi-species atoms, total electron-phonon interaction parameter should be expressed as $\lambda = \sum_m \lambda_m$ with $\lambda_m = \eta_m/M_m\langle\omega_m^2\rangle$ the electron-phonon interaction parameters for every species atoms. If the phonon modes correlated with the vibrations of oxygen atoms have most significant contributions to superconductivity, we can get simple relation $M\langle\omega^2\rangle\lambda = \eta = const$. Additionally, we assume it is correct for isotope substitution, when mass of oxygen atom increases from 16 a.u to 18 a.u. Both λ and $\langle\omega^2\rangle$ should be changed to keep $M\langle\omega^2\rangle\lambda = \eta = const$.

The Fig. (1) plots the $\Delta-\Omega$ relation for the samples with ^{16}O and ^{18}O. Certainly, the products $M\langle\omega^2\rangle\lambda$ are all the same for all the points in the Fig. (1)(a). The curve for ^{18}O are beneath the curve for ^{16}O. The very similar result is found in Fig.5(a) in Ref. [3]. The energy-gaps decrease with increasing phonon energy Ω_P because the parameters of electron-phonon interaction increase with decreasing phonon energy because $M\langle\omega^2\rangle\lambda = const$. In a sample of superconductor, the in-homogeneously distributed phonon-energies $\Omega_P(r)$ lead to the in-homogeneously distributed energy-gap $\Delta(\omega,r)$, where Ω_P is large, $\Delta(\omega,r)$ small. The vertical shift of $\Delta-\Omega_P$ curve downward to smaller value for larger mass is due to the increasing parameter of electron-phonon interaction with decreasing Mass because of the relation $M\langle\omega^2\rangle\lambda = const$. However, the energy gaps Δ in this work are only about half of values in Ref. [3] and the vertical shift of 4.0 meV in Δ smaller than 5.6 meV in Ref. [3]. The reason is that the energy gaps in this paper are directly correlated to the formation of coherent cooper pairs and the energy gaps in Ref. [3] are the mixing of superconducting gap and pseudo-gap of spin fluctuations. The values of superconducting energy gap is about from 23 meV larger than the values 19-20 meV in this work. The effects of the relationship $M\langle\omega^2\rangle\lambda = const$ had already been discussed in Ref.[9, 10].

A T_C map on the parameters space $\lambda-\Omega-\mu^*$ is very helpful to understand the superconductivity with electron-phonon mechanism. The important role of the relationship $M\langle\omega^2\rangle\lambda = const$ can be shown clearly on the T_C map. In this paper we provide T_C maps on 2-dimensional $\lambda-\Omega$ plane with 50× 50 mesh-grid with parameters λ from 0.5 to 4.0 and Ω_P from 0 meV to 80 meV. We plot two different T_C maps with the Coulomb pseudo-potential μ^*=0.1 Fig. (2) and 0.24 Fig. (3). For every mesh points we can calculate a T_C using imaginary-energy Matsubara methods. An important point is that, for high energy phonon mode which is the vibrations of relatively light oxygen atoms, only intermediate $\lambda(\leq 2.0)$ or intermediate electron-phonon coupling interaction can guarantee the values of T_C within the range of HTSC materials. As we expect that for large Coulomb pseudo-potential μ^*=0.24 the larger parameters λ of electron-phonon interaction are needed to obtained the same T_C for the general values μ^*=0.1.

In two figures we also plot two curves of $\Omega_P^2\lambda$=320 and 3600 (meV)^2. We have been ignored the changes of mass of atoms in the relation $M\langle\omega^2\rangle\lambda = const$. We

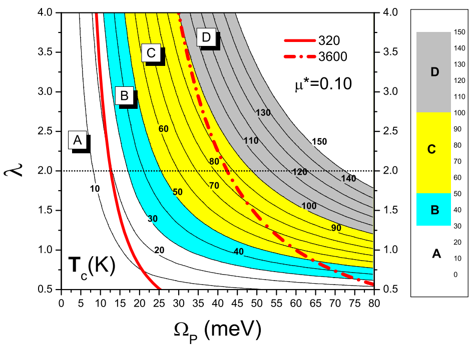

FIG. 2: The T_C map on $\lambda - \Omega_p$ plane with μ^*=0.10 obtained from imaginary-energy Matsubara method. The bold solid line and dash-dot line are the curves $\lambda\Omega_P^2$=320 and 3600 (meV)^2. The region A includes the contour lines from 0 K to 30K, B from 30 K to 50 K, C from 50 K to 100 K and D from 100 K to 150 K.

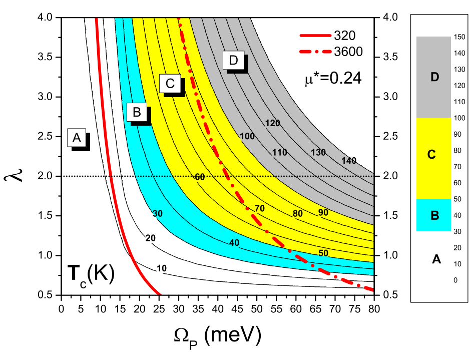

FIG. 3: The T_C map on $\lambda - \Omega_p$ plane with μ^*=0.24 obtained from imaginary-energy Matsubara method. The bold solid line and dash-dot line are the curves $\lambda\Omega_P^2$=320 and 3600 (meV)^2

can see that the two curves cross smaller number contours lines when $\lambda > 2.0$ with small phonon energies. This fact indicates that product $\langle\omega^2\rangle\lambda$ is an important parameters characterized T_C. Additionally, the curve for $\Omega_P^2\lambda$= 3600 (meV)^2 enters the region with higher transition temperature compared with the curve for $\Omega_P^2\lambda$= 320 (meV)^2. Although the range of $\lambda > 2.0$ is unfavorable superconductivity due to the lattice instability, the product is still good parameters characterized T_C. When superconductor under small structural modifications or isotope substitution, the corresponding parameters λ and Ω_P move alone these curves because the chemical environments keep almost unchanged.

For high-energy phonon, the smaller change of λ can induce large change of T_C because the curve $\Omega_P^2\lambda$=3600 cross more contour-lines than for low-energy phonon.

TABLE I: Transition temperatures T_C calculated from the real-energy method T_C^{Re} and imaginary-energy Matsubara method T_C^{Im}. The relative errors $e = (T_C^{Re} - T_C^{Im})/T_C^{av}$, where $T_C^{av} = (T_C^{Re} + T_C^{Im})/2$

	$\Omega_p(meV)$	μ^*	λ	$T_C^{Re}(K)$	$T_C^{Im}(K)$	e
(1)	25	0.10	0.8	14	15	0.069
(2)	25	0.10	1.5	33	37	0.114
(3)	25	0.24	1.8	34	39	0.137
(4)	25	0.24	2.0	38	43	0.123
(5)	52	0.10	0.8	33	35	0.059
(6)	52	0.10	1.5	79	82	0.037
(7)	52	0.24	1.8	79	86	0.085
(8)	52	0.24	2.0	90	95	0.054

So the superconductivity correlated with high-energy phonon is structural sensitivity. The energy of phonon plays more important role for high-temperature superconductor. Because the atoms with smaller mass have larger frequency of vibrations, almost all superconducting materials with high transition temperature contain light atoms such as Carbon atoms in fullerides and oxygen atom in HTSC materials. However these materials face the problem of instability of superconductivity induced by the structural instability.

The T_C values obtained using two different methods (real-energy and imaginary methods) only have small differences with relative errors $e < 0.14$ if the high-energy cutoff is larger than 1000 meV and the low-energy cutoff is smaller than 1.20 meV. In the real-energy method, the energy cutoff is about 1000 meV at high energy and 1.20 meV at low energy. In imaginary method, we use about 200 Matsubara energies to resolve the Eliashbeg equation. From the table (I) the larger relative errors happen at strong coupling regime with larger Coulomb pseudo-potentials and however with smaller phonon energies such as the case(2,3,4). With increasing the energies of phonon from 25 meV to 52 meV, the relative errors will smaller than 0.1. The absolute values of errors from 5K to 7K for the case (6,7,8) are small for high transition temperature T_C however large for the case (3,4) with relative low transition temperatures. From above comparisons, we can say that the T_C map in Fig. (2) is helpfully although there are some uncertain from the numerical calculations.

In summary, we find the anti-correlation between energy-gap Δ and phonon energy Ω_P is deduced from the simple relation $M\langle\omega^2\rangle\lambda = const$ in strong coupling theory. We also plot two T_C maps in $\lambda - \Omega_P$ to understand the above relation and the superconductivity. This work is supported by Knowledge Innovation Program of Hefei Institutes of Physical Sciences, Chinese Academy of Sciences, and in part by National Science Foundation of China for CAS projects.

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